Constructing analysis-suitable parameterization of computational domain from CAD boundary by variational harmonic method

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Abstract

In isogeometric anlaysis, parameterization of computational domain has great effects as mesh generation in finite element analysis. In this paper, based on the concept of harmonic mapping from the computational domain to parametric domain, a variational harmonic approach is proposed to construct analysis-suitable parameterization of computational domain from CAD boundary for 2D and 3D isogeometric applications. Different from the previous elliptic mesh generation method in finite element analysis, the proposed method focus on isogeometric version, and converts the elliptic PDE into a nonlinear optimization problem, in which a regular term is integrated into the optimization formulation to achieve more uniform and orthogonal isoparametric structure near convex (concave) parts of the boundary. Several examples are presented to show the efficiency of the proposed method in 2D and 3D isogeometric analysis.

Keywords: isogeometric analysis; grid generation; harmonic mapping; variational method ; analysis-suitable parameterization

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1. Introduction

The isogeometric analysis (IGA for short) method proposed by Hughes et al. in [20] is a new computational approach that offers the possibility of seamless integration between CAD and CAE. The method uses the same type of mathematical representation (spline representation), both for the geometry and for the physical solutions, and thus avoids this costly forth and back transformations. Moreover its reduces the number of parameters needed to describe the geometry, which is of particular interest for shape optimization.

Mesh generation, which generates a discrete grid of a computational domain from a given CAD object, is a key and the most time-consuming step in finite element analysis (FEA for short). It consumes about 80% of the overall design and analysis process [6] in automotive, aerospace and ship industry. Parametrization of computational domain in IGA, which corresponds to the mesh generation in FEA, also has some impact on analysis result and efficiency. In particular, arbitrary refinements can be performed on the computational mesh in FEA, but in IGA if we compute with tensor product B-splines, we can only perform refinement operations in each parametric direction by knot insertion or degree elevation. Hence, parameterization of computational domain is also being important for IGA. As it is pointed by Cottrell et al.[9], one of the most significant challenges towards isogeometric analysis is constructing analysis-suitable parameterizations from given CAD boundary representation.

In IGA, the parameterization of a computational domain is determined by control points, knot vectors and the degrees of B-spline objects. For 2D and 3D IGA problems, the knot vectors and the degree of the computational domain are determined by the given boundary curves/surfaces. That is, given boundary curves/surfaces, the quality of parameterization of computational domain is determined by the positions of inner control points. Hence, finding a good placement of the inner control points inside the computational domain, is a key issue. As the required mesh quality in FEA [28][29][30], a basic requirement of the resulting parameterization for IGA is that it doesn't have self-intersections, so that it is an injective map from the parametrization domain to the computational domain.

In the field of mesh generation in FEA, a general method is based on partial differential equations [27]. The grid points are the solution of an elliptic partial differential equation system with Dirichlet boundary conditions on all boundaries. There are several advantages in elliptic mesh generation. The theory of partial differential equations guarantees that the mapping between physical and transformed regions will be one-to-one. Another important property is the inherent smoothness in the solution of elliptic systems. A disadvantage of elliptic method is that there will be some non-uniform grid elements near convex (concave) parts of the boundary. Moreover, special treatment should be considered to achieve orthogonal mesh[42][41][33].

Motivated from the elliptic grid generation method in FEA, in this paper, we study the analysis-suitable parameterization problem of computational domain in isogeometric analysis. Our main contributions are:

- A nonlinear optimization framework based on harmonic mapping theory is proposed to generate a analysis-suitable parameterization of computational domain without self-intersections for 2D and 3D isogeometric applications.
- A regular term is integrated into the optimization formulation to achieve more uniform and orthogonal isoparametric structure near convex (concave) parts of the boundary.
- We test the parameterization results on 2D and 3D heat conduction problems to show the effectiveness of the proposed method.

The remainder of the paper is organized as follows. Section 2 reviews the related work in IGA. Section 3 describes the variational harmonic method for analysis-suitable parameterization of 2D computational domain. The 3D case for volume parameterization is studied in Section 4. Some examples and comparisons based on the isogeometric heat conduction problem are presented in Section 5. Finally, we conclude this paper and outline future works in Section 6.

2. Related work

In this section, we will review some related works in IGA and parameterization of computational domains.

IGA was firstly proposed by Hughes et al. [20] in 2005 to achieve the seamless integration of CAD and FEA. Since then, many researchers in the fields of computational mechanical and geometric computation were involved in this topic. The current work on isogeometric analysis can be classified into four categories: (1) application of IGA to various simulation and analysis problems [3][5][11][19][12][26]; (2) application of various modeling tools such as T-splines and PHT-splines in geometric computation to IGA [6] [13] [7] [24] [25] [31]; (3) accuracy and efficiency improvement of IGA framework by reparameterization and refinement operations [1] [4] [8] [10] [16][36][37]; (4) construction of analysis-suitable computational domain from boundary information [1][37][22] [23] [32][39][40][38].

The topic of this paper belongs to the forth field. From the viewpoint of graphics applications, volume parameterization of 3D models has been studied in [21, 35, 34]. As far as we know, there are only a few work on the parametrization of computational domains from the viewpoint of isogeometric applications. Martin et al. [22] proposed a method to fit a genus-0 triangular mesh by B-spline volume parameterization, based on discrete volumetric harmonic functions; this can be used to build computational domains for 3D IGA problems. A variational approach for constructing NURBS parameterization of swept volumes is proposed by Aigner et al [1]. Many free-form shapes in CAD systems, such as blades of turbines and propellers, are covered by this kind of volumes. Cohen et.al. [8] proposed the concept of *analysis-aware modeling*, in which the parameters of CAD models should be selected to facilitate isogeometric analysis. They also demonstrated the influence of parameterization of computational domains by several examples. Escobar et al. proposed a method to construct a trivariate T-spline volume of complex genus-zero solids for isogeometric application by using an adaptive tetrahedral meshing and mesh untangling technique [15]. However, the obtained solid T-splines have elements with negative Jacobians at the Gauss quadrature points. Zhang et al. proposed a robust and efficient algorithm to construct injective solid T-splines for genus-zero geometry from a boundary triangulation [39]. Based on the Morse theory, a volumetric parameterization method of mesh model with arbitrary topology is proposed in [32]. The above proposed methods demand a surface triangulation as input data. For the CAD boundary with spline representation, r-refinement method for generating optimal analysis-aware parameterization of computational domain is proposed based on shape optimization method [36][37]. However, it only works for specified analysis problems. In [38], a constraint optimization framework is proposed to obtain analysis-suitable volume parameterization of computational domain. Zhang et al. studied the construction of conformal solid T-spline from boundary T-spline representation by octree structure and boundary offset [40]. In this paper, based on the harmonic mapping theory, we propose a general method to construct analysis-suitable parameterization of computational domain from given CAD boundary information.

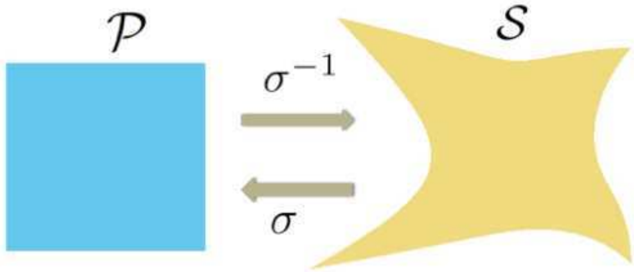


Fig. 1. The mapping σ from physical domain $\mathcal{S}$ to parametric domain $\mathcal{P}$.

3. Variational harmonic method for planar parameterization of 2D computational domain

3.1. Problem statement

Consider a simply connected bounded domain $\mathcal{S}$ in two dimensional space with Cartesian coordinates $(x;y)^T$. Suppose that $\mathcal{S}$ is bounded by four B-spline curves $\mathcal{S}(\xi,0)$, $\mathcal{S}(\xi,1)$, $\mathcal{S}(1,\eta)$ $\mathcal{S}(0,\eta)$. The parametric domain $\mathcal{P}$ of $\mathcal{S}$ should be a rectangular in two dimensional space with coordinates ξ,η, which is determined by the knot vector of boundary B-spline curves in ξ and η direction. The mapping from parametric space $\mathcal{P}$ to physical space $\mathcal{S}$ can be described as a B-spline surface $\mathcal{S}(\xi,\eta)=(x(\xi,\eta),y(\xi,\eta))=\sum_{i=0}^{n}\sum_{j=0}^{m}N_i^p(\xi)N_j^q(\eta)\boldsymbol{P}_{i,j}$ with given four B-spline curves as boundaries. $N_i^p(\xi)$ and $N_j^q(\eta)$ are B-spline basis functions, $\boldsymbol{P}_{i,j}$ are control points. Assume that this mapping is prescribed which maps the boundary of $\mathcal{P}$ one-to-one on the boundary of $\mathcal{S}$. The parameterization problem of computational domain can be stated as: given four boundary B-spline curves, find the placement of inner control points such that the resulted planar B-spline surface is a good computational domain for isogeometric analysis.

3.2. Harmonic mapping and variational harmonic function

Harmonic mapping, which is a one-to-one transformation both for 2D and 3D regions, will be used in our parameterization method. Let $\sigma:\mathcal{S}\mapsto\mathcal{P}$ be a harmonic mapping from $\mathcal{S}$ to $\mathcal{P}$. From the theory of harmonic mapping, the inverse mapping $\sigma^{-1}:\mathcal{P}\mapsto\mathcal{S}$ should be one-to-one (see Fig.1 as an example). In this section, we will convert the harmonic conditions into some constraints the inner control points of planar B-spline parameterization should satisfy.

Suppose that $\sigma:\mathcal{S}\mapsto\mathcal{P}$ is a harmonic mapping, that is

$$\Delta\xi(x,y)=\xi_{xx}+\xi_{yy}=0$$

$$\Delta\eta(x,y) = \eta_{xx} + \eta_{yy} = 0$$

By chain rules, we have

$$d\xi = \xi_x dx + \xi_y dy = \xi_x(x_\xi d\xi + x_\eta d\eta) + \xi_y(y_\xi d\xi + y_\eta d\eta)$$

$$d\eta = \eta_x dx + \eta_y dy = \eta_x(x_\xi d\xi + x_\eta d\eta) + \eta_y(y_\xi d\xi + y_\eta d\eta)$$

From above two equation, we have

$$\xi_x x_\xi + \xi_y y_\xi = \eta_x x_\eta + \eta_y y_\eta = 1 \tag{1}$$

$$\xi_x x_\eta + \xi_y y_\eta = \eta_x x_\xi + \eta_y y_\xi = 0 \tag{2}$$

By solving above two linear systems, we obtain

$$\xi_x = \frac{y_\eta}{J}, \xi_y = \frac{-x_\eta}{J}, \eta_x = \frac{-y_\xi}{J}, \eta_y = \frac{x_\xi}{J}$$

where

$$J = x_\xi y_\eta - x_\eta y_\xi$$

is Jacobian of transformation from $\mathcal{P}$ to $\mathcal{S}$.

From above results and $\frac{\partial}{\partial x} = \xi_x \frac{\partial}{\partial \xi}$, $\frac{\partial}{\partial y} = \xi_y \frac{\partial}{\partial \xi}$, we have

$$\begin{aligned} J\Delta\xi(x,y) &= J\frac{\partial}{\partial x}\xi_x + J\frac{\partial}{\partial y}\xi_y \\ &= (J\xi_x \frac{\partial}{\partial \xi} + J\eta_x \frac{\partial}{\partial \eta})\xi_x + (J\xi_y \frac{\partial}{\partial \xi} + J\eta_y \frac{\partial}{\partial \eta})\xi_y \\ &= (y_\eta \frac{\partial}{\partial \xi} - y_\xi \frac{\partial}{\partial \eta})(\frac{y_\xi}{J}) + (-x_\eta \frac{\partial}{\partial \xi} + x_\xi \frac{\partial}{\partial \eta})(\frac{-x_\eta}{J}) = 0 \end{aligned}$$

After differential computation, we have

$$-y_\eta Lx + x_\eta Ly = 0$$

where

$$L = (x_\eta^2 + y_\eta^2)\frac{\partial^2}{\partial \xi^2} - 2(x_\xi x_\eta + y_\xi y_\eta)\frac{\partial^2}{\partial \xi \eta} + (x_\xi^2 + y_\xi^2)\frac{\partial^2}{\partial \eta^2}$$

Similarly, from $J\Delta\eta(x,y) = 0$, we have

$$y_\xi Lx - x_\xi Ly = 0$$

Then we obtain

$$Lx(\xi,\eta) = Ly(\xi,\eta) = 0$$

that is,

$$\| L\mathcal{S}(\xi,\eta) \|^2 = (Lx)^2 + (Ly)^2 = 0$$

This is a nonlinear system in terms of inner control points of the planar B-spline parameterization. The final grid obtained by this method usually has non-uniform elements near convex(concave) boundary region. In order to solve this problem and achieve a grid with good orthogonality, we minimize the following energy function as in [37]

$$\begin{aligned} &\iint \lambda_1(\| \mathcal{S}_{\xi\xi} \|^2 + \| \mathcal{S}_{\eta\eta} \|^2 + 2 \| \mathcal{S}_{\xi\eta} \|^2) \\ &+\lambda_2(\| \mathcal{S}_{\xi} \|^2 + \| \mathcal{S}_{\eta} \|^2) dudv \end{aligned}$$

Then by adding the harmonic mapping term into above energy function, we obtain a new energy function for parameterization of computational domain

$$\begin{aligned} &\iint \| L\mathcal{S}(\xi,\eta) \|^2 + \lambda_1(\| \mathcal{S}_{\xi\xi} \|^2 + \| \mathcal{S}_{\eta\eta} \|^2 \\ &+2 \| \mathcal{S}_{\xi\eta} \|^2) + \lambda_2(\| \mathcal{S}_{\xi} \|^2 + \| \mathcal{S}_{\eta} \|^2) dudv \end{aligned} \tag{3}$$

where λ_1 and λ_2 are positive weights to control the final parameterization results.

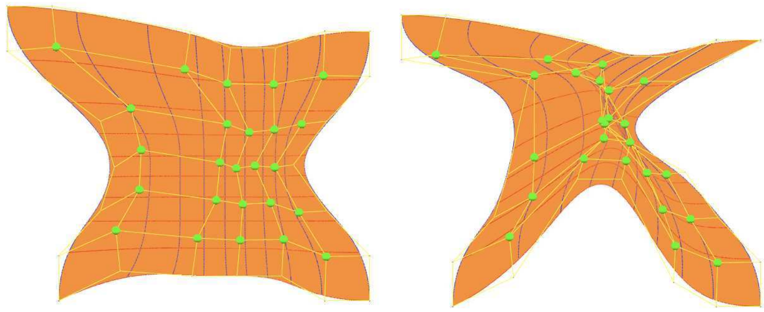
The Discrete Coons method is used to construct initial inner control points, and the Steepest Descent method is employed to minimize the energy function. The details will be described in the following two subsections.

3.3. Initial construction of inner control points

In order to solve this constraint optimization problem, an initial construction of inner control points is required. We rely on the discrete Coons method presented in [17] to generate inner control points as initial value from boundary control points. See Fig. 2 (a) for an example.

Given the boundary control points $\boldsymbol{P}_{0,j}, \boldsymbol{P}_{n,j}, \boldsymbol{P}_{i,0}$, $\boldsymbol{P}_{i,m}$, $i = 0,\dots,n, j = 0,\dots,m$, the inner control points $\boldsymbol{P}_{i,j}$ $(i = 1,\dots,n-1, j = 1,\dots,m-1)$ can be constructed by the discrete Coons method as follows:

$$\begin{aligned} \boldsymbol{P}_{i,j} &= (1-\frac{i}{n})\boldsymbol{P}_{0,j} + \frac{i}{n}\boldsymbol{P}_{n,j} + (1-\frac{j}{m})\boldsymbol{P}_{i,0} + \frac{j}{m}\boldsymbol{P}_{i,m} \\ &\quad -[1-\frac{i}{n} \quad \frac{i}{n}] \begin{bmatrix} \boldsymbol{P}_{0,0} & \boldsymbol{P}_{0,m} \\ \boldsymbol{P}_{n,0} & \boldsymbol{P}_{n,m} \end{bmatrix} \begin{bmatrix} 1-\frac{j}{m} \\ \frac{j}{m} \end{bmatrix} \end{aligned}$$



(a) (b)

Fig. 2. Examples of B-spline surface constructed by discrete Coons method: (a) example without self-intersection ; (b) example with self-intersections. Green control points are inner control points to be constructed.

Since the sum of the coefficients equals 1, the resulting inner control points lie in the convex hull of the boundary control points. For some given boundary curves, this construction may cause some self-intersections, and lead to an improper parameterization for IGA. See Fig. 2 (b) for such an example.

3.4. Optimization method

In the proposed approach, we minimize the objective function (3) , by moving inner control points of the computational domain. Therefore, we consider as optimization variables the coordinates of the inner control points and as cost function the error of the IGA solution. The optimization algorithm used for this study is a classical steepest-descent method in conjunction with a back-tracking line-search. For this exercise, the gradient of the cost function is approximated using a centered finite-differencing scheme.

Each iteration k of the optimization algorithm can be summarized as follows, starting from a point x_k in the variable space:

1. Evaluation of perturbed points $x_k + \epsilon e_k$
2. Estimation of the gradient $\nabla f(x_k)$ by finite-difference
3. Define search direction $d_k = -\nabla f(x_k)$
4. Line search : find ρ such as $f(x_k + \rho d_k) < f(x_k)$

These steps are carried out until a stopping criterion is satisfied.

3.5. Overview of variational harmonic method

In general, the proposed variational harmonic method can be summerized as follows:

Input: four coplanar boundary B-spline curves

Output: inner control points and the corresponding planar B-spline surfaces

- Construct the initial inner control points by discrete Coons method as shown in subsection 3.3;
- Solve the following optimization problem by using steepest-descent method

$$\mathbf{Min} \iint \| L\mathcal{S}(\xi,\eta) \|^2 + \lambda_1(\| \mathcal{S}_{\xi\xi} \|^2 + \| \mathcal{S}_{\eta\eta} \|^2$$
$$+2 \| \mathcal{S}_{\xi\eta} \|^2) + \lambda_2(\| \mathcal{S}_{\xi} \|^2 + \| \mathcal{S}_{\eta} \|^2) dudv$$

- Generate the corresponding planar B-spline surface $\mathcal{S}(\xi,\eta)$ as computational domain.

4. Variational harmonic method for volume parameterization of 3D computational domain

In this section, we will study the volume parameterization problem by variational harmonic method. Suppose that $\mathcal{S}$ is a simply connected bounded domain in three dimensional space with Cartesian coordinates $(x; y; z)^T$, and is bounded by six B-spline surfaces $\mathcal{S}(\xi,0,\zeta), \mathcal{S}(\xi,1,\zeta), \mathcal{S}(1,\eta,\zeta), \mathcal{S}(0,\eta,\zeta), \mathcal{S}(\xi,\eta,0), \mathcal{S}(\xi,\eta,1)$. The parametric domain $\mathcal{P}$ of $\mathcal{S}$ should be a cube in three dimensional space with coordinates ξ,η,ζ, which is determined by the knot vector of boundary B-spline surfaces in ξ, η and ζ direction. The mapping from parametric space $\mathcal{P}$ to physical space $\mathcal{S}$ can be described as a B-spline volume $\mathcal{S}(\xi,\eta,\zeta) = (x(\xi,\eta,\zeta), y(\xi,\eta,\zeta), z(\xi,\eta,\zeta)) = \sum_{i=0}^{n}\sum_{j=0}^{m}\sum_{k=0}^{l} N_i^p(\xi)\, N_j^q(\eta) N_k^r(\zeta) \boldsymbol{P}_{i,j,k}$ with given six B-spline surfaces as boundaries. $N_i^p(\xi)$, $N_j^q(\eta)$ and $N_k^r(\zeta)$ are B-spline basis functions, $\boldsymbol{P}_{i,j,k}$ are control points. Assume that this mapping is prescribed which maps the boundary of $\mathcal{P}$ one-to-one on the boundary of $\mathcal{S}$. The volume parameterization problem of 3D computational domain can be stated as: given six boundary B-spline surfaces, find the placement of inner control points such that the resulted trivariate B-spline parametric volume is a good computational domain for 3D isogeometric analysis.

4.1. Harmonic mapping and variational harmonic function

Similar with the 2D case, the harmonic conditions in 3D case will be converted into some constraints the inner control points of trivariate B-spline volume parameterization should satisfy.

If the mapping $\sigma : \mathcal{S} \mapsto \mathcal{P}$ is a harmonic mapping, we have

$$\Delta\xi(x,y,z) = \xi_{xx} + \xi_{yy} + \xi_{zz} = 0$$

$$\Delta\eta(x,y,z) = \eta_{xx} + \eta_{yy} + \eta_{zz} = 0$$

$$\Delta\zeta(x,y,z) = \zeta_{xx} + \zeta_{yy} + \zeta_{zz} = 0$$

By chain rules, we have

$$d\xi = \xi_x dx + \xi_y dy + \xi_z dz = \xi_x(x_\xi d\xi + x_\eta d\eta + x_\zeta d\zeta)$$
$$+\xi_y(y_\xi d\xi + y_\eta d\eta + y_\zeta d\zeta) + \xi_z(z_\xi d\xi + z_\eta d\eta + z_\zeta d\zeta)$$

$$d\eta = \eta_x dx + \eta_y dy + \eta_z dz = \eta_x (x_\xi d\xi + x_\eta d\eta + x_\zeta d\zeta)$$
$$+\eta_y (y_\xi d\xi + y_\eta d\eta + y_\zeta d\zeta) + \eta_z (z_\xi d\xi + z_\eta d\eta + z_\zeta d\zeta)$$

$$d\zeta = \zeta_x dx + \zeta_y dy + \zeta_z dz = \zeta_x (x_\xi d\xi + x_\eta d\eta + x_\zeta d\zeta)$$
$$+\zeta_y (y_\xi d\xi + y_\eta d\eta + y_\zeta d\zeta) + \zeta_z (z_\xi d\xi + z_\eta d\eta + z_\zeta d\zeta)$$

From above three equation, we have

$$\begin{aligned} \xi_x x_\xi + \xi_y y_\xi + \xi_z z_\xi &= 1 \\ \eta_x x_\eta + \eta_y y_\eta + \eta_z z_\eta = \zeta_x x_\zeta + \zeta_y y_\zeta + \zeta_z z_\zeta &= 1 \\ \xi_x x_\eta + \xi_y y_\eta + \xi_z z_\eta = \eta_x x_\xi + \eta_y y_\xi + \eta_z z_\xi &= 0 \\ \xi_x x_\zeta + \xi_y y_\zeta + \xi_z z_\zeta = \zeta_x x_\xi + \zeta_y y_\xi + \zeta_z z_\xi &= 0 \\ \eta_x x_\zeta + \eta_y y_\zeta + \eta_z z_\zeta = \zeta_x x_\eta + \zeta_y y_\eta + \zeta_z z_\eta &= 0 \end{aligned}$$

By solving above three linear systems, we obtain

$$\begin{aligned} \xi_x &= \frac{y_\eta z_\zeta - y_\zeta z_\eta}{J}, \xi_y = -\frac{x_\eta z_\zeta - x_\zeta z_\eta}{J}, \xi_z = \frac{y_\eta z_\zeta - y_\zeta z_\eta}{J}, \\ \eta_x &= \frac{y_\xi z_\zeta - y_\zeta z_\xi}{J}, \eta_y = -\frac{x_\xi z_\zeta - x_\zeta z_\xi}{J}, \eta_z = \frac{y_\xi z_\zeta - y_\zeta z_\xi}{J}, \\ \zeta_x &= \frac{y_\eta z_\xi - y_\xi z_\eta}{J}, \zeta_y = -\frac{x_\eta z_\xi - x_\xi z_\eta}{J}, \zeta_z = \frac{y_\eta z_\xi - y_\xi z_\eta}{J}, \end{aligned}$$

where

$$J = \begin{vmatrix} x_\xi & y_\xi & z_\xi \\ x_\eta & y_\eta & z_\eta \\ x_\zeta & y_\zeta & z_\zeta \end{vmatrix}$$

is Jacobian of transformation from $\mathcal{P}$ to $\mathcal{S}$.

From above results and $J\Delta\xi(x,y,z) = 0$,$J\Delta\eta(x,y,z) = 0$, $J\Delta\zeta(x,y,z) = 0$, the following condition can be derived,

$$Lx(\xi,\eta,\zeta) = Ly(\xi,\eta,\zeta) = Lz(\xi,\eta,\zeta) = 0 \tag{4}$$

where

$$L = a^{11}\frac{\partial^2}{\partial\xi^2} + 2a^{12}\frac{\partial^2}{\partial\xi\eta} + 2a^{13}\frac{\partial^2}{\partial\xi\zeta} + a^{22}\frac{\partial^2}{\partial\eta^2} + 2a^{23}\frac{\partial^2}{\partial\eta\zeta} + a^{33}\frac{\partial^2}{\partial\zeta^2},$$

$$\begin{aligned} a^{11} &= a_{22}a_{33} - a_{23}^2, & a^{12} &= a_{13}a_{23} - a_{12}a_{33}, \\ a^{13} &= a_{12}a_{23} - a_{13}a_{22}, & a^{22} &= a_{11}a_{33} - a_{13}^2, \\ a^{23} &= a_{13}a_{12} - a_{11}a_{23}, & a^{33} &= a_{11}a_{22} - a_{12}^2, \end{aligned}$$

and

$$a_{11} = (\mathcal{S}_\xi, \mathcal{S}_\xi), a_{12} = (\mathcal{S}_\xi, \mathcal{S}_\eta), a_{13} = (\mathcal{S}_\xi, \mathcal{S}_\zeta),$$
$$a_{22} = (\mathcal{S}_\eta, \mathcal{S}_\eta), a_{23} = (\mathcal{S}_\eta, \mathcal{S}_\zeta), a_{33} = (\mathcal{S}_\zeta, \mathcal{S}_\zeta).$$

Eq. (4) can be rewritten as

$$\| L\mathcal{S}(\xi, \eta, \zeta) \|^2 = (Lx)^2 + (Ly)^2 + (Lz)^2 = 0$$

Similarly with the 2D problem, it is also a nonlinear system in terms of inner control points of the B-spline volume parameterization. In order to achieve uniform and orthogonal iso-parametric structure near convex(concave) boundary region, we minimize the following energy function as in [38]

$$\begin{aligned}&\iint \lambda_1(\| \mathcal{S}_{\xi\xi} \|^2 + \| \mathcal{S}_{\eta\eta} \|^2 + 2 \| \mathcal{S}_{\xi\eta} \|^2 + 2 \| \mathcal{S}_{\eta\zeta} \|^2 + \\ &2 \| \mathcal{S}_{\xi\zeta} \|^2 + \| \mathcal{S}_{\zeta\zeta} \|^2) + \lambda_2(\| \mathcal{S}_\xi \|^2 + \| \mathcal{S}_\eta \|^2 + \| \mathcal{S}_\zeta \|^2) dudv\end{aligned}$$

A new energy function for volume parameterization of computational domain can be obtained by combining the harmonic mapping term and the above energy function,

$$\begin{aligned}&\iint \| L\mathcal{S}(\xi, \eta, \zeta) \|^2 + \lambda_1(\| \mathcal{S}_{\xi\xi} \|^2 + \| \mathcal{S}_{\eta\eta} \|^2 \\ &+ 2 \| \mathcal{S}_{\xi\eta} \|^2 + 2 \| \mathcal{S}_{\eta\zeta} \|^2 + 2 \| \mathcal{S}_{\xi\zeta} \|^2 + \| \mathcal{S}_{\zeta\zeta} \|^2) \\ &+ \lambda_2(\| \mathcal{S}_\xi \|^2 + \| \mathcal{S}_\eta \|^2 + \| \mathcal{S}_\zeta \|^2) dudv \end{aligned} \tag{5}$$

where λ_1 and λ_2 are positive weights to control the final parameterization results.

4.2. Initial construction of inner control points

The initial construction of inner control points for volume parameterization is based on the discrete Coons volume generation method presented in [17] from given boundary control points.

Suppose that the given boundary surfaces are B-spline surfaces and that the opposite boundary B-spline surfaces have the same degree, number of control points and knot vectors. The interior control points $\boldsymbol{P}_{i,j,k}$

can be constructed as linear combinations of points described by the following formulas:

$$
\begin{aligned}
&\boldsymbol{P}_{i,j,k} = (1-i/l)\boldsymbol{P}_{0,j,k} + i/l\boldsymbol{P}_{l,j,k} + (1-j/m)\boldsymbol{P}_{i,0,k} \\
&+j/m\boldsymbol{P}_{i,m,k} + (1-k/n)\boldsymbol{P}_{i,j,0} + k/n\boldsymbol{P}_{i,j,n} \\
&-[1-i/l, i/l]\begin{bmatrix} \boldsymbol{P}_{0,0,k} & \boldsymbol{P}_{0,m,k} \\ \boldsymbol{P}_{l,0,k} & \boldsymbol{P}_{l,m,k} \end{bmatrix}\begin{bmatrix} 1-j/m \\ j/m \end{bmatrix} \\
&-[1-j/m, j/m]\begin{bmatrix} \boldsymbol{P}_{i,0,0} & \boldsymbol{P}_{i,0,n} \\ \boldsymbol{P}_{i,m,0} & \boldsymbol{P}_{i,m,n} \end{bmatrix}\begin{bmatrix} 1-k/n \\ k/n \end{bmatrix} \\
&-[1-k/n, k/n]\begin{bmatrix} \boldsymbol{P}_{0,j,0} & \boldsymbol{P}_{l,j,0} \\ \boldsymbol{P}_{0,j,n} & \boldsymbol{P}_{l,j,n} \end{bmatrix}\begin{bmatrix} 1-i/l \\ i/l \end{bmatrix} \\
&+(1-k/n)\left[[1-i/l, i/l]\begin{bmatrix} \boldsymbol{P}_{0,0,0} & \boldsymbol{P}_{0,m,0} \\ \boldsymbol{P}_{l,0,0} & \boldsymbol{P}_{l,m,0} \end{bmatrix}\begin{bmatrix} 1-j/m \\ j/m \end{bmatrix}\right] \\
&+k/n\left[[1-i/l, i/l]\begin{bmatrix} \boldsymbol{P}_{0,0,n} & \boldsymbol{P}_{0,m,n} \\ \boldsymbol{P}_{l,0,n} & \boldsymbol{P}_{l,m,n} \end{bmatrix}\begin{bmatrix} 1-j/m \\ j/m \end{bmatrix}\right]
\end{aligned}
$$

Then the corresponding B-spline volume has the following form

$$\mathcal{S}(\xi,\eta,\zeta) = \sum_{i=0}^{l}\sum_{j=0}^{m}\sum_{k=0}^{n} N_i^p(\xi)N_j^q(\eta)N_k^r(\zeta)\boldsymbol{P}_{i,j,k}.$$

where $N_i^p(\xi)$, $N_j^q(\eta)$ and $N_k^r(\zeta)$ are B-spline basis function with knot vectors given by boundary surfaces.

4.3. Overview

The proposed variational harmonic method for volume parameterization can be summerized as follows:

Input: six boundary B-spline surfaces

Output: inner control points and the corresponding B-spline volumes

- Construct the initial inner control points by discrete Coons method as shown in subsection 4.2;
- Solve the following optimization problem by using steepest-descent method presented in ;

$$
\begin{aligned}
&\mathbf{Min} \iint \parallel L\mathcal{S}(\xi,\eta,\zeta) \parallel^2 + \lambda_1(\parallel \mathcal{S}_{\xi\xi} \parallel^2 + \parallel \mathcal{S}_{\eta\eta} \parallel^2 \\
&+2 \parallel \mathcal{S}_{\xi\eta} \parallel^2 + 2 \parallel \mathcal{S}_{\eta\zeta} \parallel^2 + 2 \parallel \mathcal{S}_{\xi\zeta} \parallel^2 + \parallel \mathcal{S}_{\zeta\zeta} \parallel^2) \\
&+\lambda_2(\parallel \mathcal{S}_{\xi} \parallel^2 + \parallel \mathcal{S}_{\eta} \parallel^2 + \parallel \mathcal{S}_{\zeta} \parallel^2) dudv
\end{aligned}
$$

- Generate the corresponding B-spline volume $\mathcal{S}(\xi,\eta,\zeta)$ as computational domain.

5. Examples and comparison

In this section, we aim at presenting several examples to show the efficiency of the proposed method. We will also give a comparison study between the original parameterization and the final parameterization constructed by the proposed method based on the 2D and 3D heat conduction problem.

5.1. Test model — heat conduction problem

For ease of presentation, we consider the second order elliptic PDE with homogeneous Dirichlet boundary condition as an illustrative model problem :

$$\begin{aligned} -\boldsymbol{\Delta} U(\mathbf{x}) &= f(\mathbf{x}) \quad \text{in } \Omega \\ U(\mathbf{x}) &= 0 \qquad \text{on } \partial\Omega \end{aligned} \tag{6}$$

where $\mathbf{x}$ are the Cartesian coordinates, Ω is a Lipschitz domain with boundary $\partial\Omega$, $f(\mathbf{x}) \in L^2(\Omega) : \Omega \mapsto \mathbb{R}$ is a given source term, and $U(\mathbf{x}) : \Omega \mapsto \mathbb{R}$ is the unknown solution.

Starting from a planar B-spline surface (or trivariate B-spline parametric volume) as computational domain, a general framework of an isogeometric solver for 2D and 3D heat conduction problem (6) has been implemented as a plugin in the AXEL[1] platform, yielding a B-spline surface (or B-spline volume) as solution field. Additional details concerning the isogeometric solver of problem (6) can be found in [14]. The proposed variational harmonic method is implemented as a part of the isogeometric toolbox of the project EXCITING[2].

In this paper, we test the different parameterizations of computational domains for 2D heat conduction problem (6) with source term

$$\boldsymbol{f}(x, y) = \frac{4\pi^2}{9} \sin(\frac{\pi x}{3}) \sin(\frac{\pi y}{3}). \tag{7}$$

and 3D problem with source term

$$\boldsymbol{f}(x, y, z) = \frac{\pi^2}{3} \sin(\frac{\pi x}{3}) \sin(\frac{\pi y}{3}) \sin(\frac{\pi z}{3}). \tag{8}$$

For problems with unknown exact solution U, suppose that U_h is the approximation solution obtained by isogeometric method, then the discrete error $e = U - U_h$. We employ a posteriori error assessment proposed in [37] to compare the initial and final parameterization of the computational domain. It can be obtained by resolving the following problem,

$$\begin{aligned} \Delta e &= -f + \Delta U_h \quad \text{in } \Omega \\ e &= 0 \qquad\qquad \text{on } \partial\Omega_D \end{aligned} \tag{9}$$

[1] http://axel.inria.fr/

[2] http://exciting-project.eu/

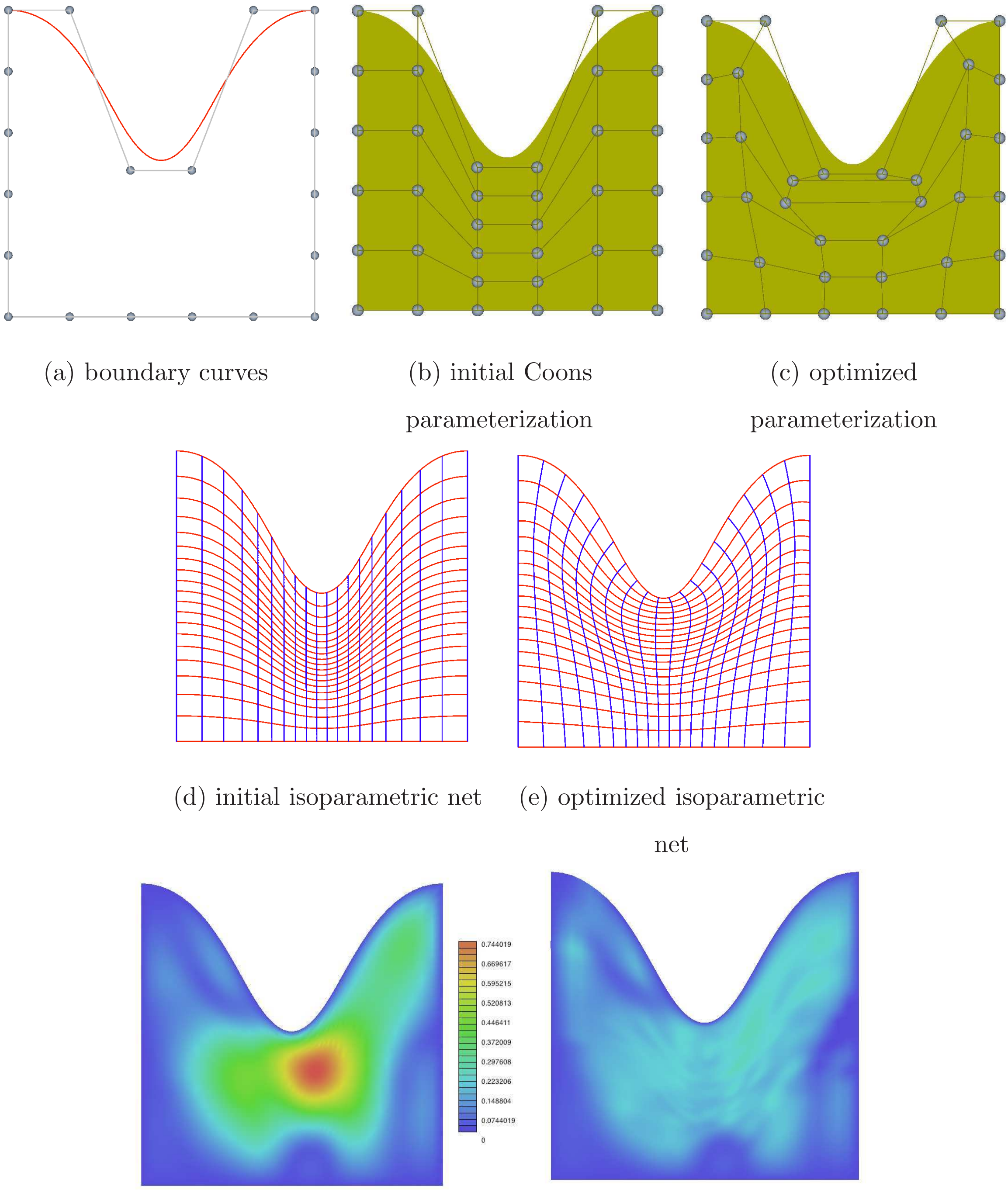
The approximation error e from (9) also has a B-spline form. Some h-refinement operation should be performed to achieve more accurate results for above problem. Though it is much more expensive, it can be used as an error assessment method to show the effectiveness of the proposed construction method of computational domain.

The first 2D example is shown in Fig. 3. Fig. 3 (a) presents the given boundary B-spline curves. Fig. 3(b) presents the initial parametrization of computational domain constructed by discrete Coons method. Fig. 3(c) shows the optimized parametrization of computational domain constructed by the proposed variational harmonic method. Fig. 3(d) and Fig. 3(e) show the isoparametric curves of the planar B-spline parameterization. We can find that the optimized parameterization has better uniformity and orthogonality than the initial parameterization. The corresponding simulation error of 2D heat conduction problem (9) for different parameterization shown in Fig. 3(a) and Fig. 3(b) are illustrated in Fig. 3 (f) and 3 (g) with the same scale.

Another 2D example is illustrated in Fig. 4. The given boundary B-spline curves is shown in Fig. 4 (a). Fig. 4(b) presents the initial parametrization of computational domain constructed by discrete Coons method. There are some self-intersections on the initial parameterization as shown by the isoparametric curves in Fig. 4(d). Fig. 4(c) shows the optimized parametrization of computational domain constructed by variational harmonic method.The optimized parameterization has no self-intersection as illustrated in Fig. 4(e).

Fig. 5 shows a 3D example, which is drawn partly to illustrate the interior information of the volume. The given boundary B-spline surfaces and curves are shown in Fig. 5 (a) and 5 (b). Fig. 5 (c) presents the initial volume parametrization of computational domain constructed by discrete Coons method. There are some self-intersections on the initial parameterization. Fig. 5 (d) shows the final volume parameterization of computational domain without self-intersections constructed by variational harmonic method. To illustrate the quality of the parameterization, the iso-parametric surfaces of the resulted B-spline volume are presented in Fig. 5 (e) and 5 (f). Fig. 5 (g) and 5 (h) presents the corresponding solution field obtained from the volume parameterization in Fig. 5 (c) and Fig. 5 (d) . Obviously, the solution field in Fig. 5 (h) is more smooth than the solution field in Fig. 5 (g), which indicates that the final volume parameterization is better than the initial one. Another 3D example with complex geometry is shown in Fig. 6.

Quantitative data of the examples presented in Fig. 3, Fig.4, Fig. 5 and Fig. 6 are summarized in Table.1. Overall, the optimized parameterization obtained by the variational harmonic method has better quality, and can achieve better simulation results than the initial Coons parameterization.



(a) boundary curves

(b) initial Coons parameterization

(c) optimized parameterization

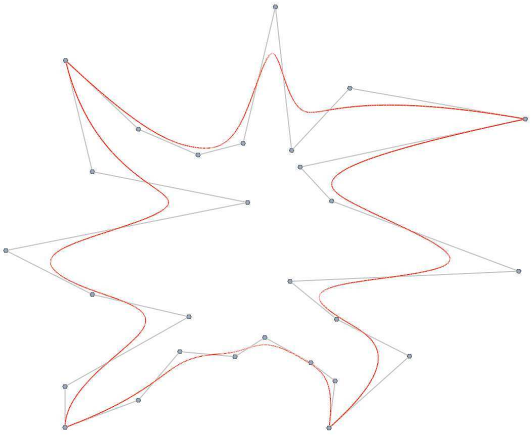
(d) initial isoparametric net

(e) optimized isoparametric net

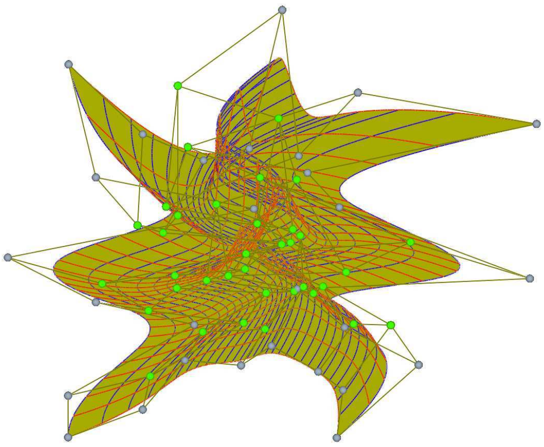
(f) simulation error w.r.t Coons parameterization

(g) simulation error w.r.t optimized parameterization with same scale

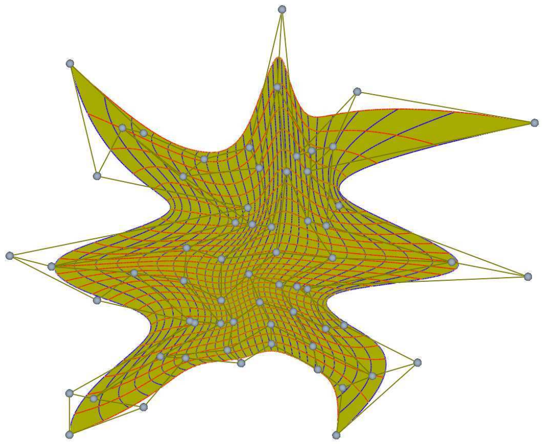
Fig. 3. 2D example I.



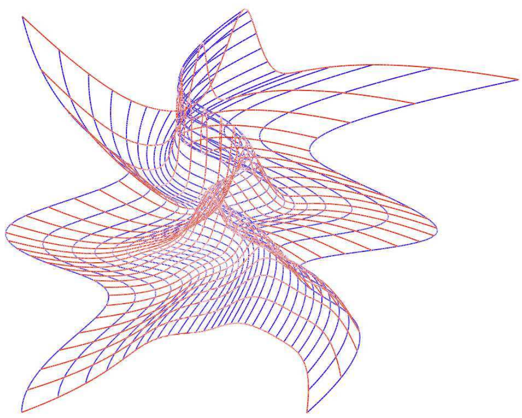
(a) boundary curves



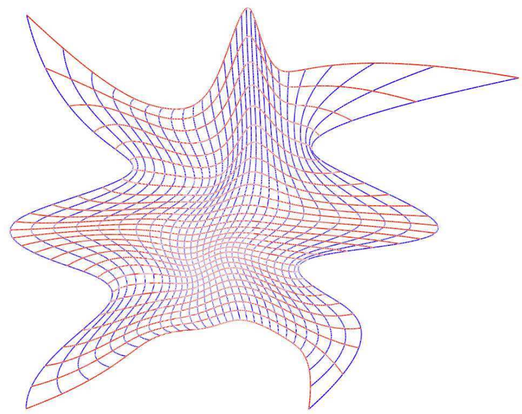
(b) initial Coons parameterization



(c) optimized parameterization



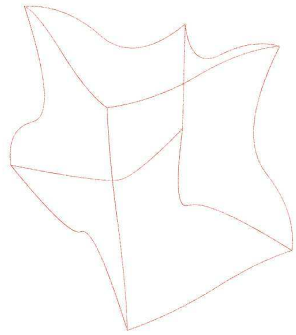
(d) initial isoparametric net



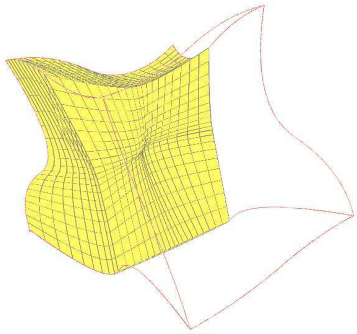
(e) optimized isoparametric net

Fig. 4. 2D example II.

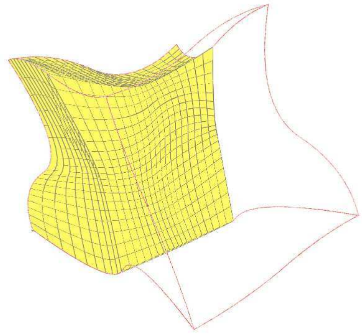
(a) boundary surfaces



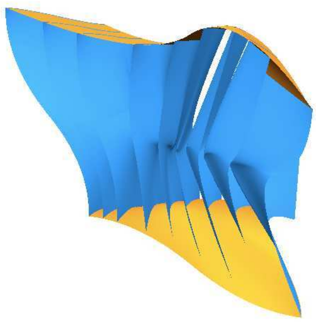
(b) boundary curves



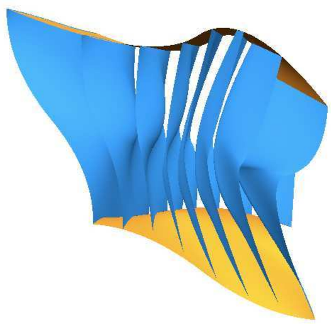
(c) Coons volume



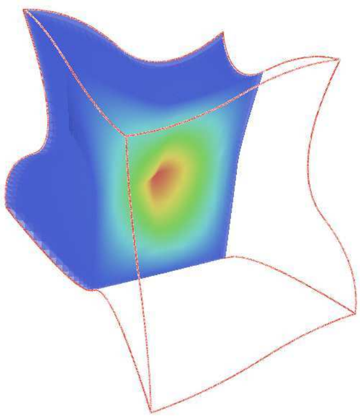
(d) optimized volume parameterization



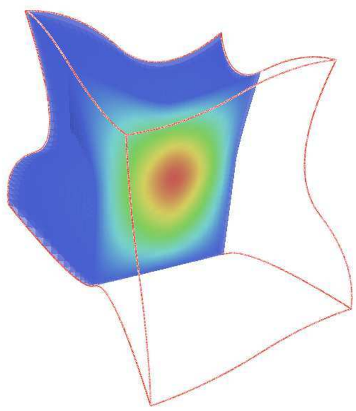
(e) initial iso-parametric surface



(f) optimized iso-parametric surface

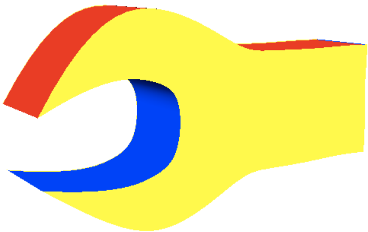


(g) solution field w.r.t Coons parameterization

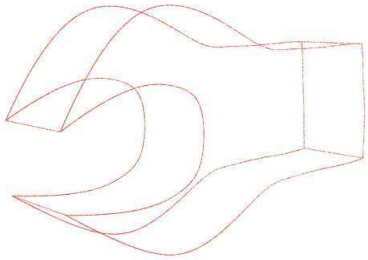


(h) solution field w.r.t optimized parameterization

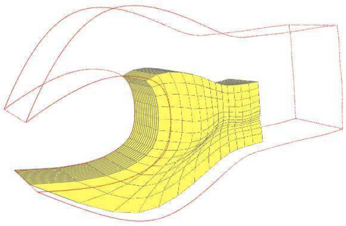
Fig. 5. 3D example I.



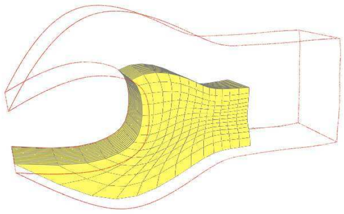
(a) boundary surfaces



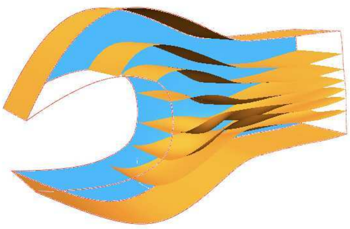
(b) boundary curves



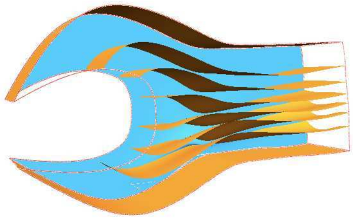
(c) Coons volume



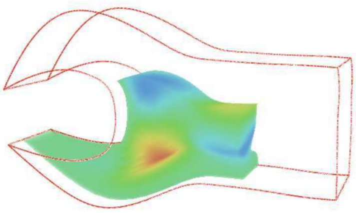
(d) optimized volume parameterization



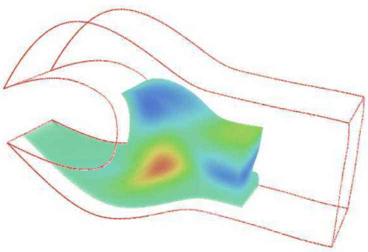
(e) initial iso-parametric surface



(f) optimized iso-parametric surface



(g) solution field w.r.t Coons parameterization



(h) solution field w.r.t optimized parameterization

Fig. 6. 3D example II.

Table 1: Quantitative data in Fig. 3, Fig.4, Fig. 5 and Fig. 6. # deg.: degree of B-spline parameterization; # con.: number of control points; # iter.: number of optimization iterations.

Example	# Deg.	# Con.	#Iter.
Fig.3	3	36	4
Fig.4	4	64	7
Fig.5	3	125	7
Fig.6	4	216	11

6. Conclusion

Parameterization of computational domain is a key point in isogeometric analysis. In this paper, we propose a variational harmonic method to parameterize the 2D and 3D computational domain from the theory of harmonic mapping. The resulted parameterization is injective and has high quality near convex(concave) parts of the boundary. Examples and comparison are presented to show that the proposed methods can produce analysis-suitable parameterization of computational domain for isogeometric analysis.

As part of the future work, we will generalize the proposed method to the computational domain with complex shape, which are more important in practice.

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